Mechanical Performance of NiFeCrMn Alloy Under Tensile Loading: An Experimental and Atomistic Model

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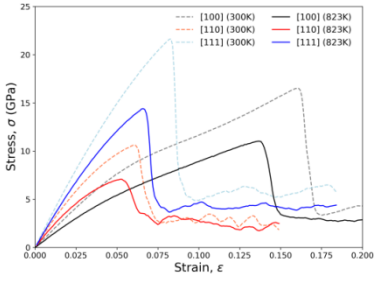
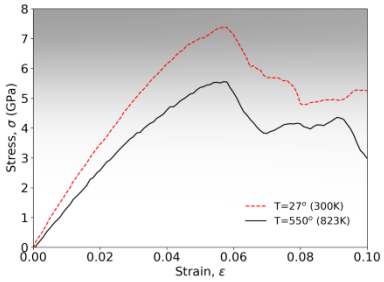
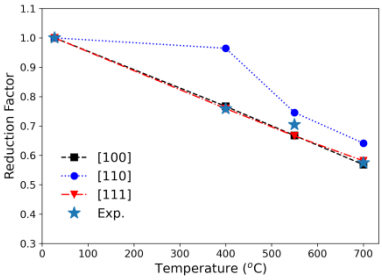
High entropy alloys (HEAs) have emerged as promising candidates for nuclear applications due to their exceptional mechanical properties, thermal stability, and resistance to radiation damage. Their unique multicomponent design enables superior performance in extreme environments, such as the high temperatures and radiation fluxes found in nuclear reactors. Among HEAs, NiFeCrMn-based alloys stand out for their high strength and ductility, making them ideal for structural materials in advanced nuclear systems. This study investigates the mechanical performance of NiFeCrMn alloy under tensile loading through atomistic computational modelling validated by experimental measurements. The work focuses on both room-temperature and high-temperature conditions, simulating single-crystal and polycrystalline samples to capture a comprehensive range of mechanical behavior. A recently developed Embedded Atom Method (EAM) potential tailored for NiFeCrMn alloys was tested and refined to ensure accuracy in representing the material's behavior across various crystallographic orientations. Careful preparation of simulated samples was performed to align closely with experimental data. Stress-strain analyses provided insights into the structural and mechanical responses, highlighting the role of temperature, grain structure, and crystal orientation on deformation mechanisms.



[1]



[2]



[3]

Fig 1-2-3. Stress-strain curve for single crystal [1] and for polycrystal [2]. Reduction factor for MD simulations and experimental data [3].

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093_abstract